wwPDB X-ray Structure Validation Summary Report (i)

Apr 4, 2024 – 12:38 PM JST

PDB ID	:	8JWK
Title	:	The second purified state crystal structure of AKRtyl
Authors	:	Lin, S.; Dai, S.; Xiao, Z.
Deposited on	:	2023-06-29
Resolution	:	2.32 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

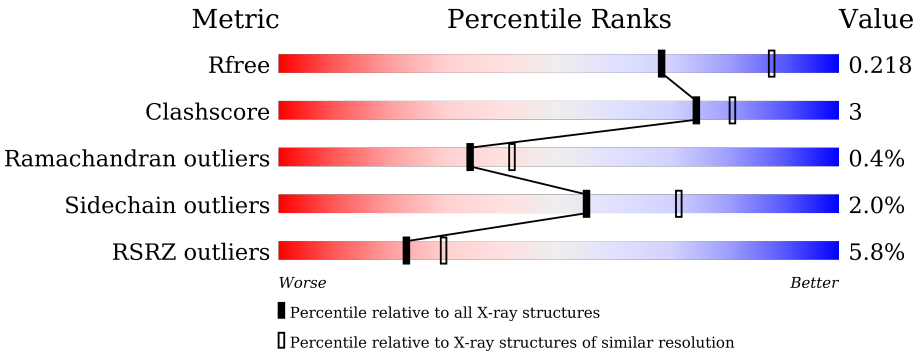
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.32 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	351	6% 79% 5% • 16%
1	B	351	8% 81% 8% • 11%
1	C	351	9% 75% 8% 17%
1	D	351	7% 81% 8% 11%
1	E	351	6% 74% 10% 16%
1	F	351	6% 79% 9% 11%

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Mol	Chain	Length	Quality of chain
1	G	351	5% 74% 10% 16%
1	H	351	4% 81% 6% 13%
1	I	351	5% 80% 6% 15%
1	J	351	5% 83% 7% 9%
1	K	351	5% 74% 9% 16%
1	L	351	4% 87% 6% 7%
1	M	351	4% 75% 9% 16%
1	N	351	3% 81% 8% 10%
1	O	351	3% 76% 8% 16%
1	P	351	4% 89% 5% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 40000 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Aldo/keto reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2309	1454	413	436	6			
1	B	312	Total	C	N	O	S	0	0	0
			2414	1522	429	455	8			
1	C	292	Total	C	N	O	S	0	0	0
			2272	1432	408	425	7			
1	D	314	Total	C	N	O	S	0	0	0
			2437	1537	435	457	8			
1	E	294	Total	C	N	O	S	0	0	0
			2288	1441	412	428	7			
1	F	313	Total	C	N	O	S	0	0	0
			2433	1533	434	458	8			
1	G	296	Total	C	N	O	S	0	0	0
			2305	1451	412	436	6			
1	H	307	Total	C	N	O	S	0	0	0
			2383	1502	425	448	8			
1	I	300	Total	C	N	O	S	0	0	0
			2333	1469	417	440	7			
1	J	321	Total	C	N	O	S	0	0	0
			2480	1558	446	468	8			
1	K	295	Total	C	N	O	S	0	0	0
			2295	1445	411	432	7			
1	L	326	Total	C	N	O	S	0	0	0
			2526	1585	457	476	8			
1	M	295	Total	C	N	O	S	0	0	0
			2298	1446	414	431	7			
1	N	315	Total	C	N	O	S	0	0	0
			2446	1542	436	460	8			
1	O	295	Total	C	N	O	S	0	0	0
			2295	1447	411	430	7			
1	P	330	Total	C	N	O	S	0	0	0
			2552	1600	462	482	8			

There are 320 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A3R7J519
A	-18	GLY	-	expression tag	UNP A0A3R7J519
A	-17	SER	-	expression tag	UNP A0A3R7J519
A	-16	SER	-	expression tag	UNP A0A3R7J519
A	-15	HIS	-	expression tag	UNP A0A3R7J519
A	-14	HIS	-	expression tag	UNP A0A3R7J519
A	-13	HIS	-	expression tag	UNP A0A3R7J519
A	-12	HIS	-	expression tag	UNP A0A3R7J519
A	-11	HIS	-	expression tag	UNP A0A3R7J519
A	-10	HIS	-	expression tag	UNP A0A3R7J519
A	-9	SER	-	expression tag	UNP A0A3R7J519
A	-8	SER	-	expression tag	UNP A0A3R7J519
A	-7	GLY	-	expression tag	UNP A0A3R7J519
A	-6	LEU	-	expression tag	UNP A0A3R7J519
A	-5	VAL	-	expression tag	UNP A0A3R7J519
A	-4	PRO	-	expression tag	UNP A0A3R7J519
A	-3	ARG	-	expression tag	UNP A0A3R7J519
A	-2	GLY	-	expression tag	UNP A0A3R7J519
A	-1	SER	-	expression tag	UNP A0A3R7J519
A	0	HIS	-	expression tag	UNP A0A3R7J519
B	-19	MET	-	initiating methionine	UNP A0A3R7J519
B	-18	GLY	-	expression tag	UNP A0A3R7J519
B	-17	SER	-	expression tag	UNP A0A3R7J519
B	-16	SER	-	expression tag	UNP A0A3R7J519
B	-15	HIS	-	expression tag	UNP A0A3R7J519
B	-14	HIS	-	expression tag	UNP A0A3R7J519
B	-13	HIS	-	expression tag	UNP A0A3R7J519
B	-12	HIS	-	expression tag	UNP A0A3R7J519
B	-11	HIS	-	expression tag	UNP A0A3R7J519
B	-10	HIS	-	expression tag	UNP A0A3R7J519
B	-9	SER	-	expression tag	UNP A0A3R7J519
B	-8	SER	-	expression tag	UNP A0A3R7J519
B	-7	GLY	-	expression tag	UNP A0A3R7J519
B	-6	LEU	-	expression tag	UNP A0A3R7J519
B	-5	VAL	-	expression tag	UNP A0A3R7J519
B	-4	PRO	-	expression tag	UNP A0A3R7J519
B	-3	ARG	-	expression tag	UNP A0A3R7J519
B	-2	GLY	-	expression tag	UNP A0A3R7J519
B	-1	SER	-	expression tag	UNP A0A3R7J519
B	0	HIS	-	expression tag	UNP A0A3R7J519
C	-19	MET	-	initiating methionine	UNP A0A3R7J519
C	-18	GLY	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-17	SER	-	expression tag	UNP A0A3R7J519
C	-16	SER	-	expression tag	UNP A0A3R7J519
C	-15	HIS	-	expression tag	UNP A0A3R7J519
C	-14	HIS	-	expression tag	UNP A0A3R7J519
C	-13	HIS	-	expression tag	UNP A0A3R7J519
C	-12	HIS	-	expression tag	UNP A0A3R7J519
C	-11	HIS	-	expression tag	UNP A0A3R7J519
C	-10	HIS	-	expression tag	UNP A0A3R7J519
C	-9	SER	-	expression tag	UNP A0A3R7J519
C	-8	SER	-	expression tag	UNP A0A3R7J519
C	-7	GLY	-	expression tag	UNP A0A3R7J519
C	-6	LEU	-	expression tag	UNP A0A3R7J519
C	-5	VAL	-	expression tag	UNP A0A3R7J519
C	-4	PRO	-	expression tag	UNP A0A3R7J519
C	-3	ARG	-	expression tag	UNP A0A3R7J519
C	-2	GLY	-	expression tag	UNP A0A3R7J519
C	-1	SER	-	expression tag	UNP A0A3R7J519
C	0	HIS	-	expression tag	UNP A0A3R7J519
D	-19	MET	-	initiating methionine	UNP A0A3R7J519
D	-18	GLY	-	expression tag	UNP A0A3R7J519
D	-17	SER	-	expression tag	UNP A0A3R7J519
D	-16	SER	-	expression tag	UNP A0A3R7J519
D	-15	HIS	-	expression tag	UNP A0A3R7J519
D	-14	HIS	-	expression tag	UNP A0A3R7J519
D	-13	HIS	-	expression tag	UNP A0A3R7J519
D	-12	HIS	-	expression tag	UNP A0A3R7J519
D	-11	HIS	-	expression tag	UNP A0A3R7J519
D	-10	HIS	-	expression tag	UNP A0A3R7J519
D	-9	SER	-	expression tag	UNP A0A3R7J519
D	-8	SER	-	expression tag	UNP A0A3R7J519
D	-7	GLY	-	expression tag	UNP A0A3R7J519
D	-6	LEU	-	expression tag	UNP A0A3R7J519
D	-5	VAL	-	expression tag	UNP A0A3R7J519
D	-4	PRO	-	expression tag	UNP A0A3R7J519
D	-3	ARG	-	expression tag	UNP A0A3R7J519
D	-2	GLY	-	expression tag	UNP A0A3R7J519
D	-1	SER	-	expression tag	UNP A0A3R7J519
D	0	HIS	-	expression tag	UNP A0A3R7J519
E	-19	MET	-	initiating methionine	UNP A0A3R7J519
E	-18	GLY	-	expression tag	UNP A0A3R7J519
E	-17	SER	-	expression tag	UNP A0A3R7J519
E	-16	SER	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-15	HIS	-	expression tag	UNP A0A3R7J519
E	-14	HIS	-	expression tag	UNP A0A3R7J519
E	-13	HIS	-	expression tag	UNP A0A3R7J519
E	-12	HIS	-	expression tag	UNP A0A3R7J519
E	-11	HIS	-	expression tag	UNP A0A3R7J519
E	-10	HIS	-	expression tag	UNP A0A3R7J519
E	-9	SER	-	expression tag	UNP A0A3R7J519
E	-8	SER	-	expression tag	UNP A0A3R7J519
E	-7	GLY	-	expression tag	UNP A0A3R7J519
E	-6	LEU	-	expression tag	UNP A0A3R7J519
E	-5	VAL	-	expression tag	UNP A0A3R7J519
E	-4	PRO	-	expression tag	UNP A0A3R7J519
E	-3	ARG	-	expression tag	UNP A0A3R7J519
E	-2	GLY	-	expression tag	UNP A0A3R7J519
E	-1	SER	-	expression tag	UNP A0A3R7J519
E	0	HIS	-	expression tag	UNP A0A3R7J519
F	-19	MET	-	initiating methionine	UNP A0A3R7J519
F	-18	GLY	-	expression tag	UNP A0A3R7J519
F	-17	SER	-	expression tag	UNP A0A3R7J519
F	-16	SER	-	expression tag	UNP A0A3R7J519
F	-15	HIS	-	expression tag	UNP A0A3R7J519
F	-14	HIS	-	expression tag	UNP A0A3R7J519
F	-13	HIS	-	expression tag	UNP A0A3R7J519
F	-12	HIS	-	expression tag	UNP A0A3R7J519
F	-11	HIS	-	expression tag	UNP A0A3R7J519
F	-10	HIS	-	expression tag	UNP A0A3R7J519
F	-9	SER	-	expression tag	UNP A0A3R7J519
F	-8	SER	-	expression tag	UNP A0A3R7J519
F	-7	GLY	-	expression tag	UNP A0A3R7J519
F	-6	LEU	-	expression tag	UNP A0A3R7J519
F	-5	VAL	-	expression tag	UNP A0A3R7J519
F	-4	PRO	-	expression tag	UNP A0A3R7J519
F	-3	ARG	-	expression tag	UNP A0A3R7J519
F	-2	GLY	-	expression tag	UNP A0A3R7J519
F	-1	SER	-	expression tag	UNP A0A3R7J519
F	0	HIS	-	expression tag	UNP A0A3R7J519
G	-19	MET	-	initiating methionine	UNP A0A3R7J519
G	-18	GLY	-	expression tag	UNP A0A3R7J519
G	-17	SER	-	expression tag	UNP A0A3R7J519
G	-16	SER	-	expression tag	UNP A0A3R7J519
G	-15	HIS	-	expression tag	UNP A0A3R7J519
G	-14	HIS	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-13	HIS	-	expression tag	UNP A0A3R7J519
G	-12	HIS	-	expression tag	UNP A0A3R7J519
G	-11	HIS	-	expression tag	UNP A0A3R7J519
G	-10	HIS	-	expression tag	UNP A0A3R7J519
G	-9	SER	-	expression tag	UNP A0A3R7J519
G	-8	SER	-	expression tag	UNP A0A3R7J519
G	-7	GLY	-	expression tag	UNP A0A3R7J519
G	-6	LEU	-	expression tag	UNP A0A3R7J519
G	-5	VAL	-	expression tag	UNP A0A3R7J519
G	-4	PRO	-	expression tag	UNP A0A3R7J519
G	-3	ARG	-	expression tag	UNP A0A3R7J519
G	-2	GLY	-	expression tag	UNP A0A3R7J519
G	-1	SER	-	expression tag	UNP A0A3R7J519
G	0	HIS	-	expression tag	UNP A0A3R7J519
H	-19	MET	-	initiating methionine	UNP A0A3R7J519
H	-18	GLY	-	expression tag	UNP A0A3R7J519
H	-17	SER	-	expression tag	UNP A0A3R7J519
H	-16	SER	-	expression tag	UNP A0A3R7J519
H	-15	HIS	-	expression tag	UNP A0A3R7J519
H	-14	HIS	-	expression tag	UNP A0A3R7J519
H	-13	HIS	-	expression tag	UNP A0A3R7J519
H	-12	HIS	-	expression tag	UNP A0A3R7J519
H	-11	HIS	-	expression tag	UNP A0A3R7J519
H	-10	HIS	-	expression tag	UNP A0A3R7J519
H	-9	SER	-	expression tag	UNP A0A3R7J519
H	-8	SER	-	expression tag	UNP A0A3R7J519
H	-7	GLY	-	expression tag	UNP A0A3R7J519
H	-6	LEU	-	expression tag	UNP A0A3R7J519
H	-5	VAL	-	expression tag	UNP A0A3R7J519
H	-4	PRO	-	expression tag	UNP A0A3R7J519
H	-3	ARG	-	expression tag	UNP A0A3R7J519
H	-2	GLY	-	expression tag	UNP A0A3R7J519
H	-1	SER	-	expression tag	UNP A0A3R7J519
H	0	HIS	-	expression tag	UNP A0A3R7J519
I	-19	MET	-	initiating methionine	UNP A0A3R7J519
I	-18	GLY	-	expression tag	UNP A0A3R7J519
I	-17	SER	-	expression tag	UNP A0A3R7J519
I	-16	SER	-	expression tag	UNP A0A3R7J519
I	-15	HIS	-	expression tag	UNP A0A3R7J519
I	-14	HIS	-	expression tag	UNP A0A3R7J519
I	-13	HIS	-	expression tag	UNP A0A3R7J519
I	-12	HIS	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-11	HIS	-	expression tag	UNP A0A3R7J519
I	-10	HIS	-	expression tag	UNP A0A3R7J519
I	-9	SER	-	expression tag	UNP A0A3R7J519
I	-8	SER	-	expression tag	UNP A0A3R7J519
I	-7	GLY	-	expression tag	UNP A0A3R7J519
I	-6	LEU	-	expression tag	UNP A0A3R7J519
I	-5	VAL	-	expression tag	UNP A0A3R7J519
I	-4	PRO	-	expression tag	UNP A0A3R7J519
I	-3	ARG	-	expression tag	UNP A0A3R7J519
I	-2	GLY	-	expression tag	UNP A0A3R7J519
I	-1	SER	-	expression tag	UNP A0A3R7J519
I	0	HIS	-	expression tag	UNP A0A3R7J519
J	-19	MET	-	initiating methionine	UNP A0A3R7J519
J	-18	GLY	-	expression tag	UNP A0A3R7J519
J	-17	SER	-	expression tag	UNP A0A3R7J519
J	-16	SER	-	expression tag	UNP A0A3R7J519
J	-15	HIS	-	expression tag	UNP A0A3R7J519
J	-14	HIS	-	expression tag	UNP A0A3R7J519
J	-13	HIS	-	expression tag	UNP A0A3R7J519
J	-12	HIS	-	expression tag	UNP A0A3R7J519
J	-11	HIS	-	expression tag	UNP A0A3R7J519
J	-10	HIS	-	expression tag	UNP A0A3R7J519
J	-9	SER	-	expression tag	UNP A0A3R7J519
J	-8	SER	-	expression tag	UNP A0A3R7J519
J	-7	GLY	-	expression tag	UNP A0A3R7J519
J	-6	LEU	-	expression tag	UNP A0A3R7J519
J	-5	VAL	-	expression tag	UNP A0A3R7J519
J	-4	PRO	-	expression tag	UNP A0A3R7J519
J	-3	ARG	-	expression tag	UNP A0A3R7J519
J	-2	GLY	-	expression tag	UNP A0A3R7J519
J	-1	SER	-	expression tag	UNP A0A3R7J519
J	0	HIS	-	expression tag	UNP A0A3R7J519
K	-19	MET	-	initiating methionine	UNP A0A3R7J519
K	-18	GLY	-	expression tag	UNP A0A3R7J519
K	-17	SER	-	expression tag	UNP A0A3R7J519
K	-16	SER	-	expression tag	UNP A0A3R7J519
K	-15	HIS	-	expression tag	UNP A0A3R7J519
K	-14	HIS	-	expression tag	UNP A0A3R7J519
K	-13	HIS	-	expression tag	UNP A0A3R7J519
K	-12	HIS	-	expression tag	UNP A0A3R7J519
K	-11	HIS	-	expression tag	UNP A0A3R7J519
K	-10	HIS	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-9	SER	-	expression tag	UNP A0A3R7J519
K	-8	SER	-	expression tag	UNP A0A3R7J519
K	-7	GLY	-	expression tag	UNP A0A3R7J519
K	-6	LEU	-	expression tag	UNP A0A3R7J519
K	-5	VAL	-	expression tag	UNP A0A3R7J519
K	-4	PRO	-	expression tag	UNP A0A3R7J519
K	-3	ARG	-	expression tag	UNP A0A3R7J519
K	-2	GLY	-	expression tag	UNP A0A3R7J519
K	-1	SER	-	expression tag	UNP A0A3R7J519
K	0	HIS	-	expression tag	UNP A0A3R7J519
L	-19	MET	-	initiating methionine	UNP A0A3R7J519
L	-18	GLY	-	expression tag	UNP A0A3R7J519
L	-17	SER	-	expression tag	UNP A0A3R7J519
L	-16	SER	-	expression tag	UNP A0A3R7J519
L	-15	HIS	-	expression tag	UNP A0A3R7J519
L	-14	HIS	-	expression tag	UNP A0A3R7J519
L	-13	HIS	-	expression tag	UNP A0A3R7J519
L	-12	HIS	-	expression tag	UNP A0A3R7J519
L	-11	HIS	-	expression tag	UNP A0A3R7J519
L	-10	HIS	-	expression tag	UNP A0A3R7J519
L	-9	SER	-	expression tag	UNP A0A3R7J519
L	-8	SER	-	expression tag	UNP A0A3R7J519
L	-7	GLY	-	expression tag	UNP A0A3R7J519
L	-6	LEU	-	expression tag	UNP A0A3R7J519
L	-5	VAL	-	expression tag	UNP A0A3R7J519
L	-4	PRO	-	expression tag	UNP A0A3R7J519
L	-3	ARG	-	expression tag	UNP A0A3R7J519
L	-2	GLY	-	expression tag	UNP A0A3R7J519
L	-1	SER	-	expression tag	UNP A0A3R7J519
L	0	HIS	-	expression tag	UNP A0A3R7J519
M	-19	MET	-	initiating methionine	UNP A0A3R7J519
M	-18	GLY	-	expression tag	UNP A0A3R7J519
M	-17	SER	-	expression tag	UNP A0A3R7J519
M	-16	SER	-	expression tag	UNP A0A3R7J519
M	-15	HIS	-	expression tag	UNP A0A3R7J519
M	-14	HIS	-	expression tag	UNP A0A3R7J519
M	-13	HIS	-	expression tag	UNP A0A3R7J519
M	-12	HIS	-	expression tag	UNP A0A3R7J519
M	-11	HIS	-	expression tag	UNP A0A3R7J519
M	-10	HIS	-	expression tag	UNP A0A3R7J519
M	-9	SER	-	expression tag	UNP A0A3R7J519
M	-8	SER	-	expression tag	UNP A0A3R7J519

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-7	GLY	-	expression tag	UNP A0A3R7J519
M	-6	LEU	-	expression tag	UNP A0A3R7J519
M	-5	VAL	-	expression tag	UNP A0A3R7J519
M	-4	PRO	-	expression tag	UNP A0A3R7J519
M	-3	ARG	-	expression tag	UNP A0A3R7J519
M	-2	GLY	-	expression tag	UNP A0A3R7J519
M	-1	SER	-	expression tag	UNP A0A3R7J519
M	0	HIS	-	expression tag	UNP A0A3R7J519
N	-19	MET	-	initiating methionine	UNP A0A3R7J519
N	-18	GLY	-	expression tag	UNP A0A3R7J519
N	-17	SER	-	expression tag	UNP A0A3R7J519
N	-16	SER	-	expression tag	UNP A0A3R7J519
N	-15	HIS	-	expression tag	UNP A0A3R7J519
N	-14	HIS	-	expression tag	UNP A0A3R7J519
N	-13	HIS	-	expression tag	UNP A0A3R7J519
N	-12	HIS	-	expression tag	UNP A0A3R7J519
N	-11	HIS	-	expression tag	UNP A0A3R7J519
N	-10	HIS	-	expression tag	UNP A0A3R7J519
N	-9	SER	-	expression tag	UNP A0A3R7J519
N	-8	SER	-	expression tag	UNP A0A3R7J519
N	-7	GLY	-	expression tag	UNP A0A3R7J519
N	-6	LEU	-	expression tag	UNP A0A3R7J519
N	-5	VAL	-	expression tag	UNP A0A3R7J519
N	-4	PRO	-	expression tag	UNP A0A3R7J519
N	-3	ARG	-	expression tag	UNP A0A3R7J519
N	-2	GLY	-	expression tag	UNP A0A3R7J519
N	-1	SER	-	expression tag	UNP A0A3R7J519
N	0	HIS	-	expression tag	UNP A0A3R7J519
O	-19	MET	-	initiating methionine	UNP A0A3R7J519
O	-18	GLY	-	expression tag	UNP A0A3R7J519
O	-17	SER	-	expression tag	UNP A0A3R7J519
O	-16	SER	-	expression tag	UNP A0A3R7J519
O	-15	HIS	-	expression tag	UNP A0A3R7J519
O	-14	HIS	-	expression tag	UNP A0A3R7J519
O	-13	HIS	-	expression tag	UNP A0A3R7J519
O	-12	HIS	-	expression tag	UNP A0A3R7J519
O	-11	HIS	-	expression tag	UNP A0A3R7J519
O	-10	HIS	-	expression tag	UNP A0A3R7J519
O	-9	SER	-	expression tag	UNP A0A3R7J519
O	-8	SER	-	expression tag	UNP A0A3R7J519
O	-7	GLY	-	expression tag	UNP A0A3R7J519
O	-6	LEU	-	expression tag	UNP A0A3R7J519

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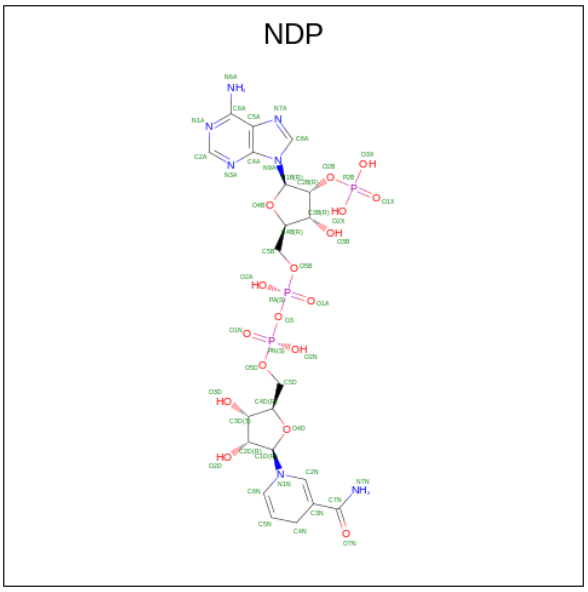
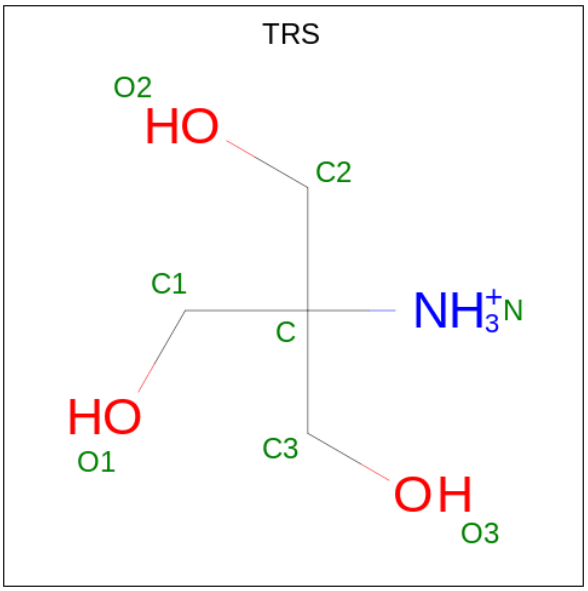
Chain	Residue	Modelled	Actual	Comment	Reference
O	-5	VAL	-	expression tag	UNP A0A3R7J519
O	-4	PRO	-	expression tag	UNP A0A3R7J519
O	-3	ARG	-	expression tag	UNP A0A3R7J519
O	-2	GLY	-	expression tag	UNP A0A3R7J519
O	-1	SER	-	expression tag	UNP A0A3R7J519
O	0	HIS	-	expression tag	UNP A0A3R7J519
P	-19	MET	-	initiating methionine	UNP A0A3R7J519
P	-18	GLY	-	expression tag	UNP A0A3R7J519
P	-17	SER	-	expression tag	UNP A0A3R7J519
P	-16	SER	-	expression tag	UNP A0A3R7J519
P	-15	HIS	-	expression tag	UNP A0A3R7J519
P	-14	HIS	-	expression tag	UNP A0A3R7J519
P	-13	HIS	-	expression tag	UNP A0A3R7J519
P	-12	HIS	-	expression tag	UNP A0A3R7J519
P	-11	HIS	-	expression tag	UNP A0A3R7J519
P	-10	HIS	-	expression tag	UNP A0A3R7J519
P	-9	SER	-	expression tag	UNP A0A3R7J519
P	-8	SER	-	expression tag	UNP A0A3R7J519
P	-7	GLY	-	expression tag	UNP A0A3R7J519
P	-6	LEU	-	expression tag	UNP A0A3R7J519
P	-5	VAL	-	expression tag	UNP A0A3R7J519
P	-4	PRO	-	expression tag	UNP A0A3R7J519
P	-3	ARG	-	expression tag	UNP A0A3R7J519
P	-2	GLY	-	expression tag	UNP A0A3R7J519
P	-1	SER	-	expression tag	UNP A0A3R7J519
P	0	HIS	-	expression tag	UNP A0A3R7J519

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	J	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	L	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	N	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	P	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total C N O 8 4 1 3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	B	70	Total O 70 70	0	0
4	C	55	Total O 55 55	0	0
4	D	110	Total O 110 110	0	0
4	E	66	Total O 66 66	0	0
4	F	90	Total O 90 90	0	0
4	G	70	Total O 70 70	0	0
4	H	97	Total O 97 97	0	0
4	I	114	Total O 114 114	0	0
4	J	144	Total O 144 144	0	0
4	K	96	Total O 96 96	0	0

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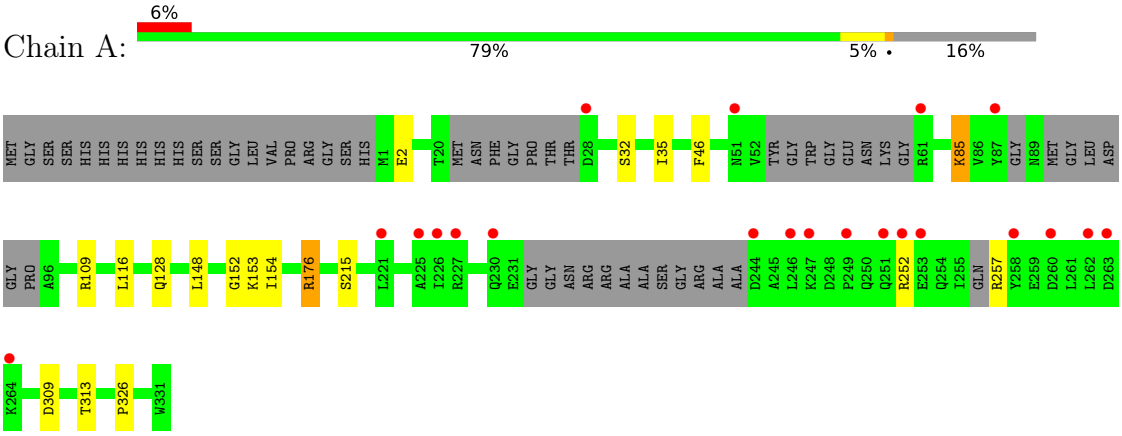
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	152	Total O 152 152	0	0
4	M	100	Total O 100 100	0	0
4	N	140	Total O 140 140	0	0
4	O	99	Total O 99 99	0	0
4	P	166	Total O 166 166	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

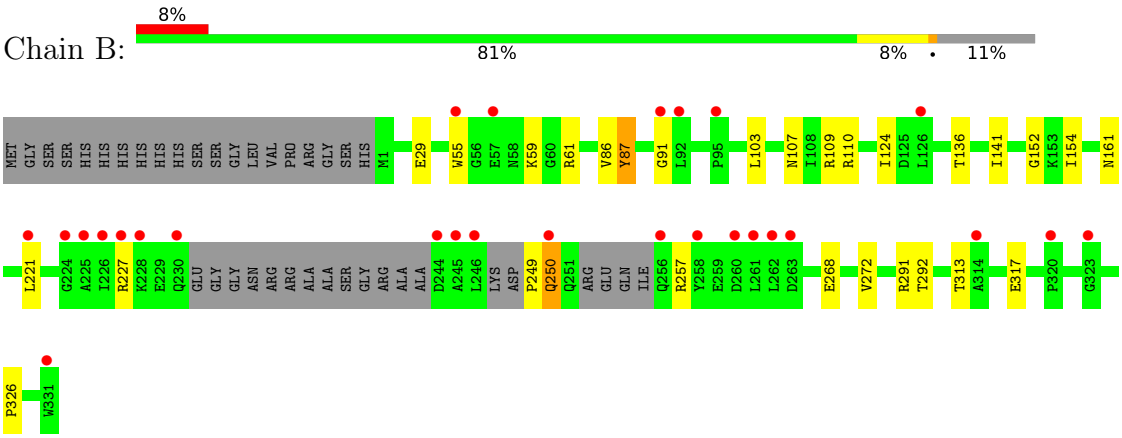
• Molecule 1: Aldo/keto reductase

Chain A:



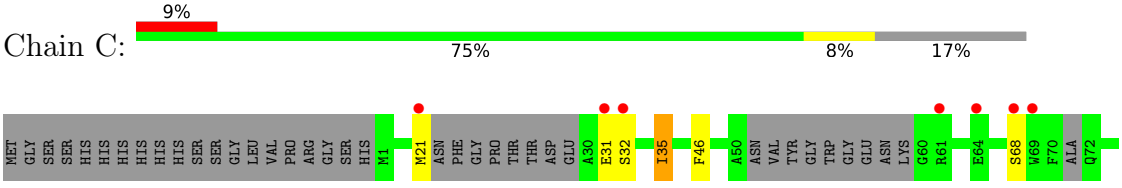
• Molecule 1: Aldo/keto reductase

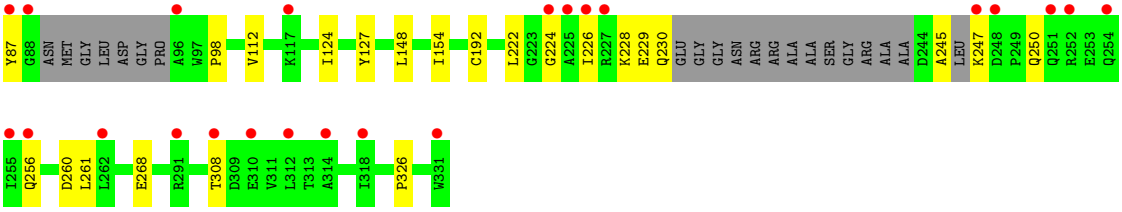
Chain B:



• Molecule 1: Aldo/keto reductase

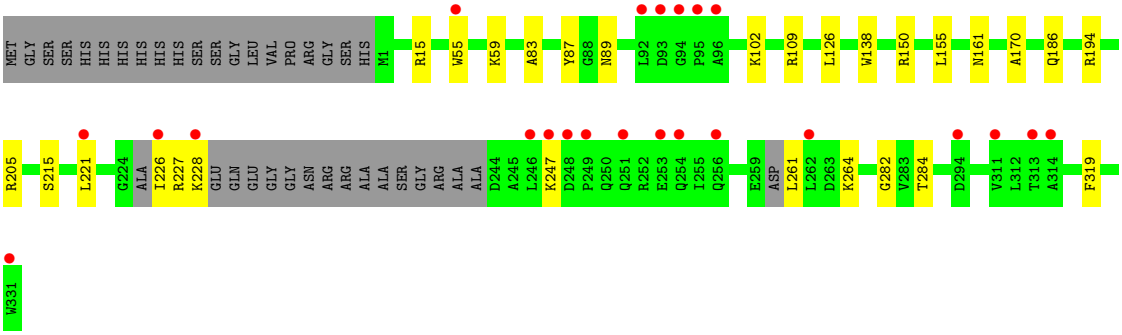
Chain C:





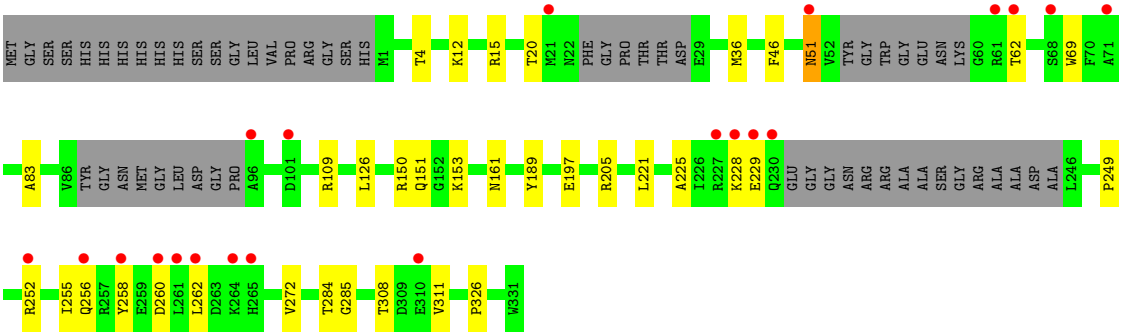
• Molecule 1: Aldo/keto reductase

Chain D:



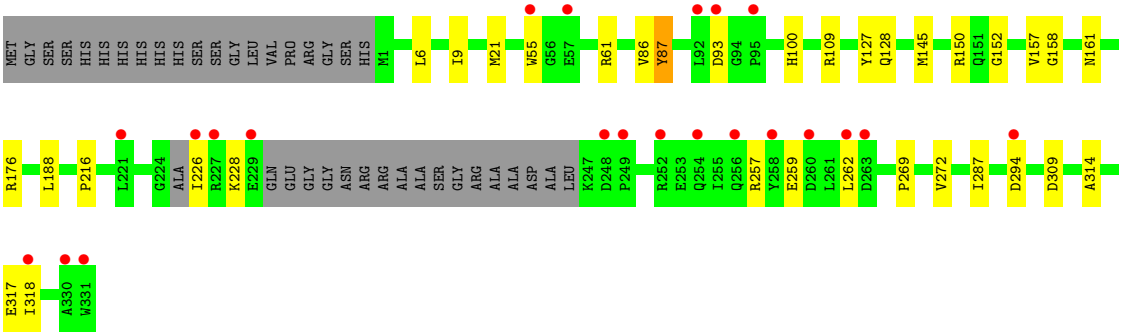
• Molecule 1: Aldo/keto reductase

Chain E:



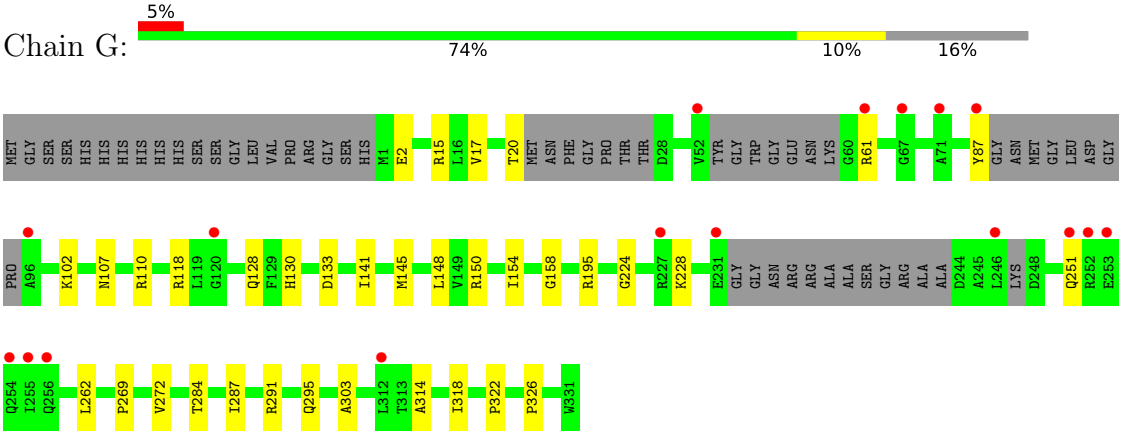
• Molecule 1: Aldo/keto reductase

Chain F:



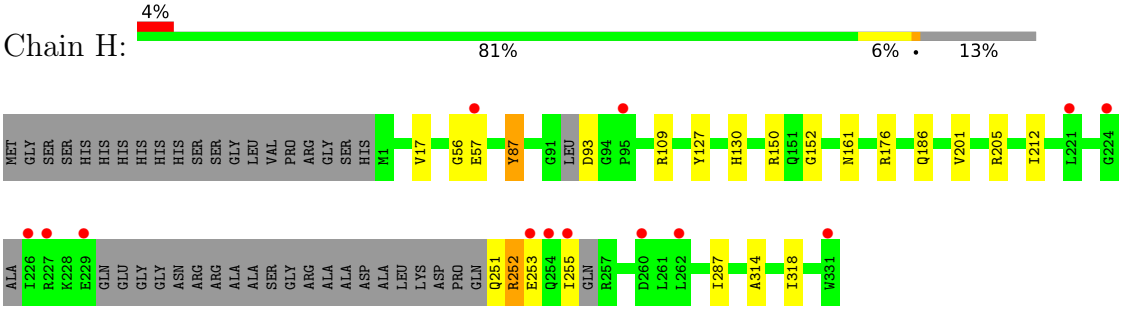
• Molecule 1: Aldo/keto reductase

Chain G:



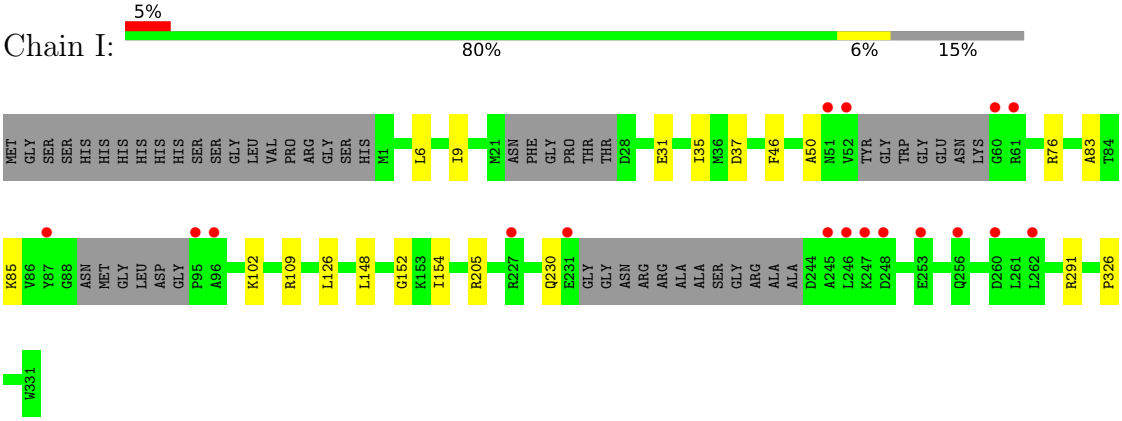
• Molecule 1: Aldo/keto reductase

Chain H:



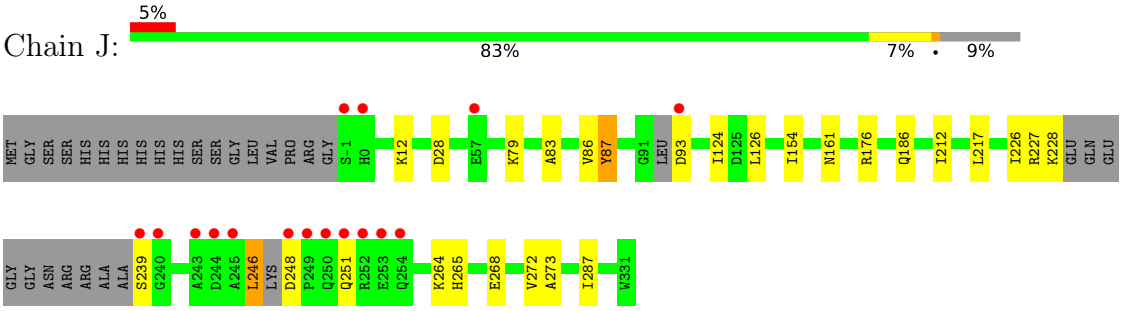
• Molecule 1: Aldo/keto reductase

Chain I:



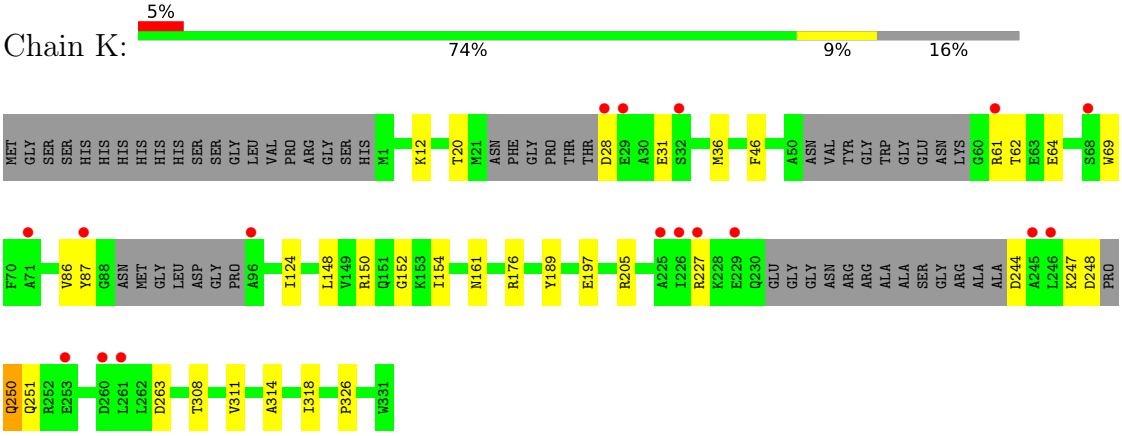
• Molecule 1: Aldo/keto reductase

Chain J:



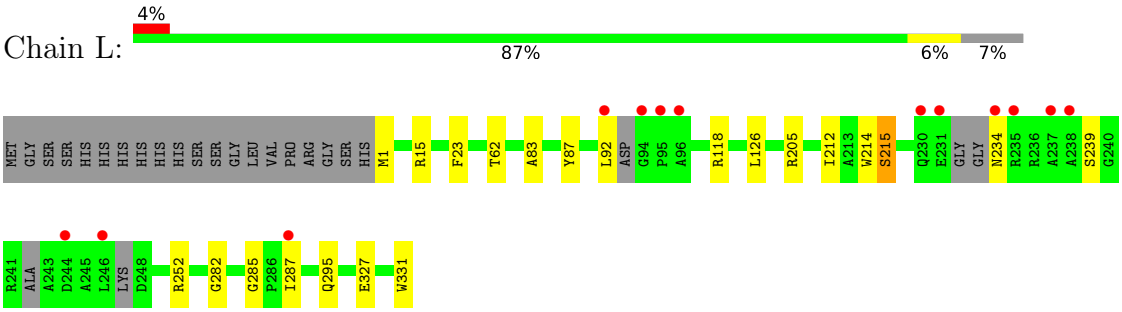
• Molecule 1: Aldo/keto reductase

Chain K:



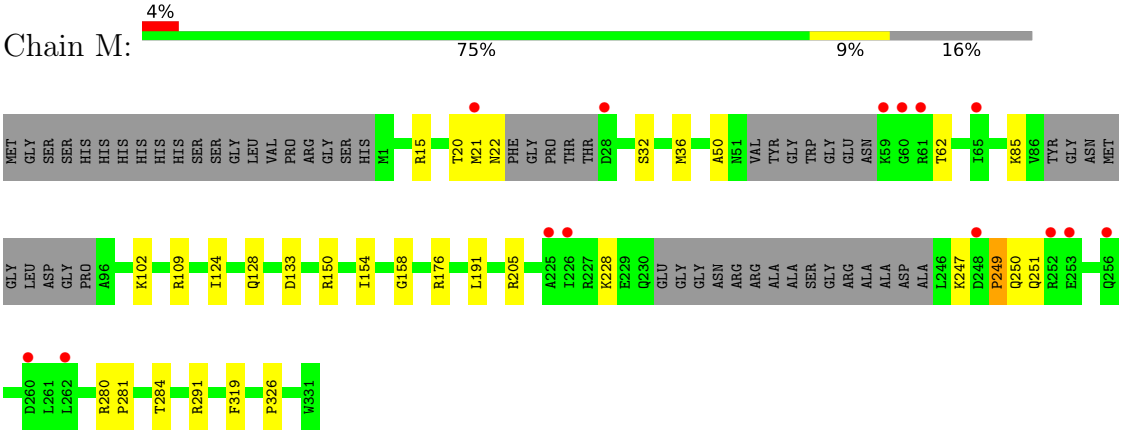
• Molecule 1: Aldo/keto reductase

Chain L:



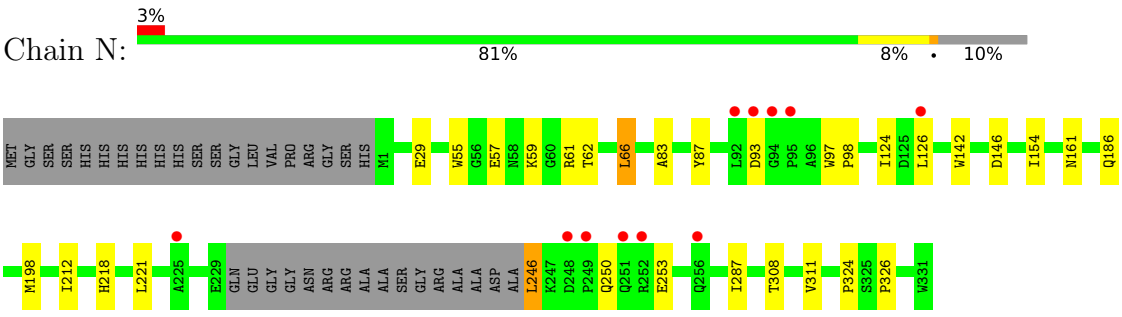
• Molecule 1: Aldo/keto reductase

Chain M:



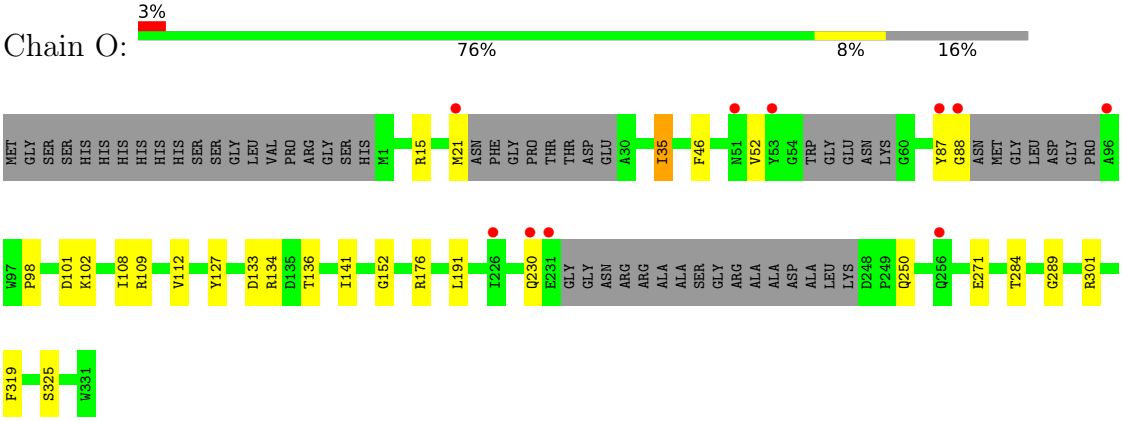
• Molecule 1: Aldo/keto reductase

Chain N:



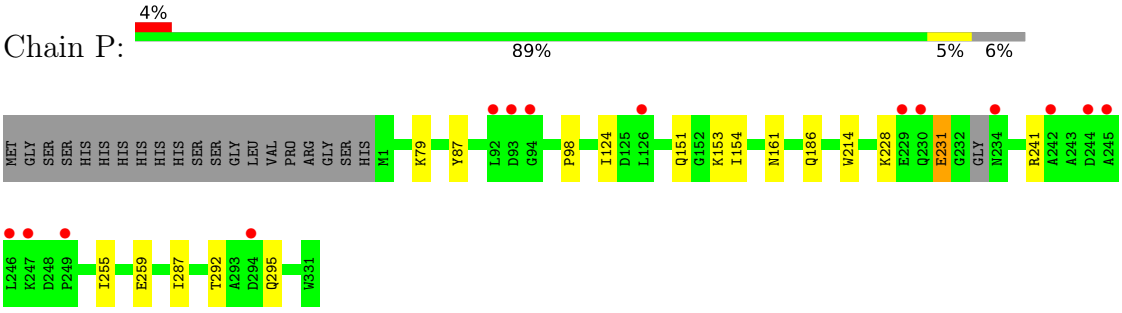
• Molecule 1: Aldo/keto reductase

Chain O:



• Molecule 1: Aldo/keto reductase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	111.89Å 111.89Å 563.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.38 – 2.32 37.77 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.38-2.32) 99.4 (37.77-2.32)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.181 , 0.217 0.181 , 0.218	Depositor DCC
R_{free} test set	14758 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	37.2	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	40000	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.14 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.1494e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, NDP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.48	0/2353	0.62	0/3189
1	B	0.44	0/2467	0.63	0/3349
1	C	0.43	0/2316	0.63	0/3136
1	D	0.43	0/2490	0.65	0/3379
1	E	0.43	0/2333	0.61	0/3163
1	F	0.43	0/2487	0.63	0/3376
1	G	0.43	0/2350	0.64	0/3187
1	H	0.47	0/2434	0.67	0/3301
1	I	0.44	0/2380	0.67	0/3227
1	J	0.47	0/2534	0.65	0/3439
1	K	0.45	0/2339	0.63	0/3168
1	L	0.48	0/2578	0.67	0/3495
1	M	0.45	0/2343	0.65	0/3175
1	N	0.45	0/2501	0.65	0/3397
1	O	0.46	0/2342	0.66	0/3176
1	P	0.46	0/2607	0.67	0/3538
All	All	0.45	0/38854	0.65	0/52695

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2309	0	2260	11	0
1	B	2414	0	2352	16	0
1	C	2272	0	2230	13	0
1	D	2437	0	2383	16	0
1	E	2288	0	2254	23	0
1	F	2433	0	2374	18	0
1	G	2305	0	2253	18	0
1	H	2383	0	2321	16	0
1	I	2333	0	2287	11	0
1	J	2480	0	2411	19	0
1	K	2295	0	2250	21	0
1	L	2526	0	2462	21	0
1	M	2298	0	2262	17	0
1	N	2446	0	2391	18	0
1	O	2295	0	2248	19	0
1	P	2552	0	2490	14	0
2	D	48	0	26	1	0
2	H	48	0	26	4	0
2	J	48	0	26	2	0
2	L	48	0	26	7	0
2	N	48	0	26	1	0
2	P	48	0	26	4	0
3	I	8	0	12	0	0
4	A	69	0	0	0	0
4	B	70	0	0	0	0
4	C	55	0	0	0	0
4	D	110	0	0	0	0
4	E	66	0	0	0	0
4	F	90	0	0	1	0
4	G	70	0	0	0	0
4	H	97	0	0	0	0
4	I	114	0	0	1	0
4	J	144	0	0	1	0
4	K	96	0	0	0	0
4	L	152	0	0	2	0
4	M	100	0	0	1	0
4	N	140	0	0	0	0
4	O	99	0	0	1	0
4	P	166	0	0	2	0
All	All	40000	0	37396	245	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 245 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:VAL:HG22	1:C:127:TYR:CZ	2.20	0.76
1:L:214:TRP:CE3	2:L:401:NDP:H41N	2.24	0.71
1:B:152:GLY:O	1:H:109:ARG:NH1	2.24	0.70
1:B:268:GLU:O	1:B:272:VAL:HG23	1.93	0.68
1:G:17:VAL:HG13	1:G:287:ILE:HA	1.74	0.68

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/351 (81%)	274 (97%)	9 (3%)	0	100	100
1	B	304/351 (87%)	289 (95%)	13 (4%)	2 (1%)	22	26
1	C	278/351 (79%)	269 (97%)	8 (3%)	1 (0%)	34	41
1	D	306/351 (87%)	294 (96%)	9 (3%)	3 (1%)	15	17
1	E	284/351 (81%)	276 (97%)	7 (2%)	1 (0%)	34	41
1	F	307/351 (88%)	294 (96%)	11 (4%)	2 (1%)	22	26
1	G	284/351 (81%)	274 (96%)	10 (4%)	0	100	100
1	H	297/351 (85%)	287 (97%)	8 (3%)	2 (1%)	22	26
1	I	290/351 (83%)	282 (97%)	8 (3%)	0	100	100
1	J	313/351 (89%)	300 (96%)	11 (4%)	2 (1%)	25	30
1	K	283/351 (81%)	276 (98%)	7 (2%)	0	100	100
1	L	316/351 (90%)	305 (96%)	10 (3%)	1 (0%)	41	50
1	M	285/351 (81%)	276 (97%)	7 (2%)	2 (1%)	22	26
1	N	311/351 (89%)	296 (95%)	13 (4%)	2 (1%)	25	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	O	285/351 (81%)	277 (97%)	8 (3%)	0	100 100
1	P	326/351 (93%)	315 (97%)	10 (3%)	1 (0%)	41 50
All	All	4752/5616 (85%)	4584 (96%)	149 (3%)	19 (0%)	34 41

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	249	PRO
1	J	227	ARG
1	M	249	PRO
1	B	87	TYR
1	D	87	TYR

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	237/275 (86%)	231 (98%)	6 (2%)	47 64
1	B	246/275 (90%)	242 (98%)	4 (2%)	62 77
1	C	232/275 (84%)	222 (96%)	10 (4%)	29 40
1	D	249/275 (90%)	244 (98%)	5 (2%)	55 71
1	E	235/275 (86%)	233 (99%)	2 (1%)	78 89
1	F	249/275 (90%)	241 (97%)	8 (3%)	39 53
1	G	236/275 (86%)	232 (98%)	4 (2%)	60 75
1	H	243/275 (88%)	237 (98%)	6 (2%)	47 64
1	I	239/275 (87%)	236 (99%)	3 (1%)	69 81
1	J	252/275 (92%)	247 (98%)	5 (2%)	55 71
1	K	234/275 (85%)	228 (97%)	6 (3%)	46 62
1	L	256/275 (93%)	251 (98%)	5 (2%)	55 71
1	M	236/275 (86%)	232 (98%)	4 (2%)	60 75
1	N	250/275 (91%)	247 (99%)	3 (1%)	71 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	O	234/275 (85%)	227 (97%)	7 (3%)	41 56
1	P	258/275 (94%)	257 (100%)	1 (0%)	91 96
All	All	3886/4400 (88%)	3807 (98%)	79 (2%)	55 71

5 of 79 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	250	GLN
1	O	21	MET
1	L	92	LEU
1	M	247	LYS
1	O	230	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	O	177	HIS
1	P	234	ASN
1	F	254	GLN
1	K	186	GLN
1	M	22	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

7 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NDP	N	401	-	45,52,52	0.77	0	53,80,80	0.90	2 (3%)
2	NDP	P	401	-	45,52,52	0.67	0	53,80,80	1.02	3 (5%)
2	NDP	J	401	-	45,52,52	0.68	0	53,80,80	0.98	2 (3%)
3	TRS	I	401	-	7,7,7	0.41	0	9,9,9	0.59	0
2	NDP	D	401	-	45,52,52	0.70	0	53,80,80	0.84	1 (1%)
2	NDP	H	401	-	45,52,52	0.69	0	53,80,80	0.86	0
2	NDP	L	401	-	45,52,52	0.75	1 (2%)	53,80,80	0.88	1 (1%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	N	401	-	-	3/30/77/77	0/5/5/5
2	NDP	P	401	-	-	2/30/77/77	0/5/5/5
2	NDP	J	401	-	-	5/30/77/77	0/5/5/5
3	TRS	I	401	-	-	9/9/9/9	-
2	NDP	D	401	-	-	5/30/77/77	0/5/5/5
2	NDP	H	401	-	-	3/30/77/77	0/5/5/5
2	NDP	L	401	-	-	3/30/77/77	0/5/5/5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	401	NDP	P2B-O2B	2.45	1.63	1.59

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	P	401	NDP	O3B-C3B-C2B	3.01	119.71	111.17
2	N	401	NDP	C5A-C6A-N6A	2.68	124.43	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	J	401	NDP	C5A-C6A-N6A	2.65	124.38	120.35
2	J	401	NDP	O2B-P2B-O1X	-2.63	99.22	109.39
2	P	401	NDP	C5A-C6A-N6A	2.40	124.00	120.35

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	NDP	C2B-O2B-P2B-O1X
2	H	401	NDP	C5B-O5B-PA-O2A
2	J	401	NDP	C2B-O2B-P2B-O1X
2	L	401	NDP	C2B-O2B-P2B-O2X
2	N	401	NDP	C2B-O2B-P2B-O1X

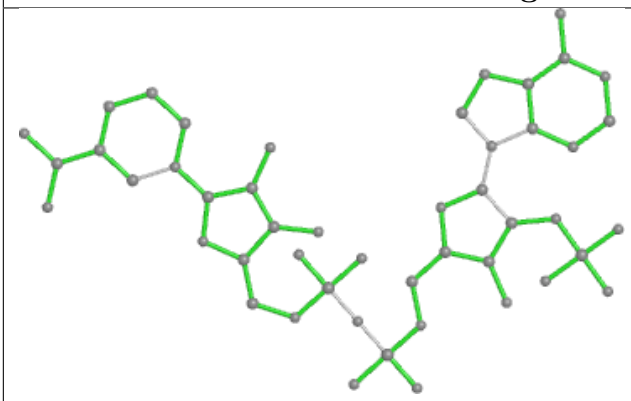
There are no ring outliers.

6 monomers are involved in 19 short contacts:

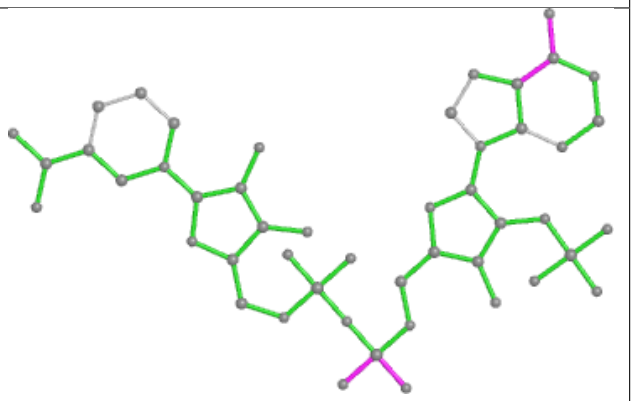
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	401	NDP	1	0
2	P	401	NDP	4	0
2	J	401	NDP	2	0
2	D	401	NDP	1	0
2	H	401	NDP	4	0
2	L	401	NDP	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

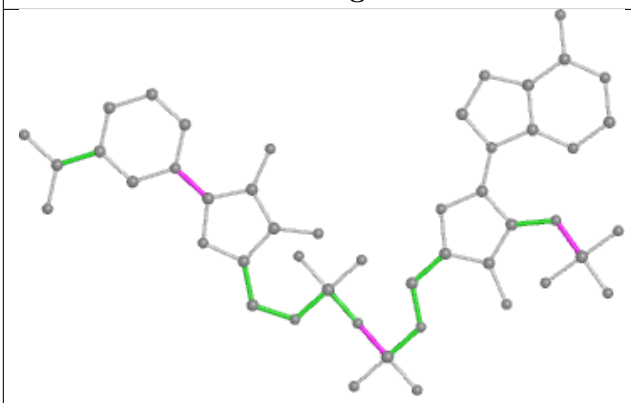
Ligand NDP N 401



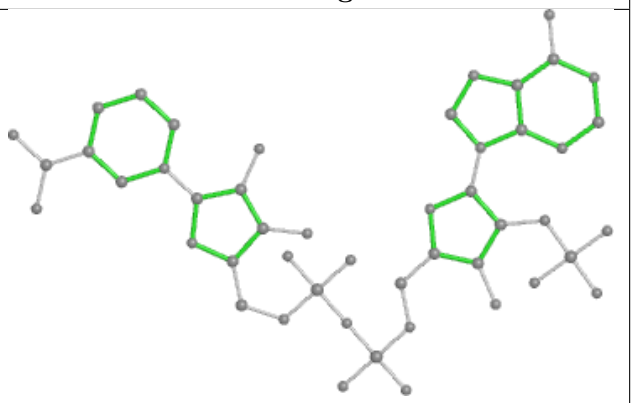
Bond lengths



Bond angles

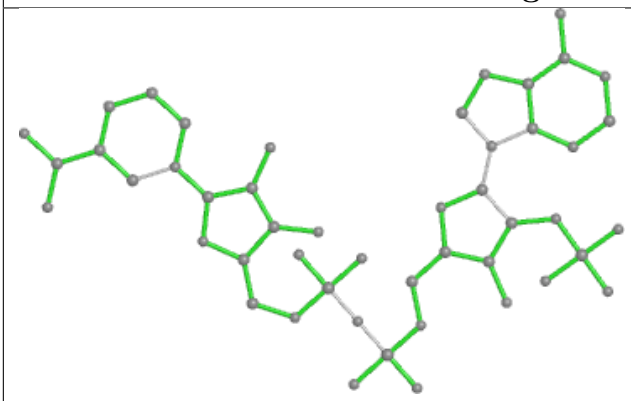


Torsions



Rings

Ligand NDP P 401



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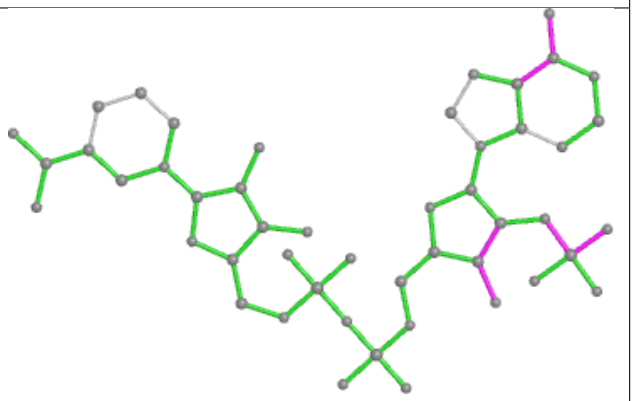

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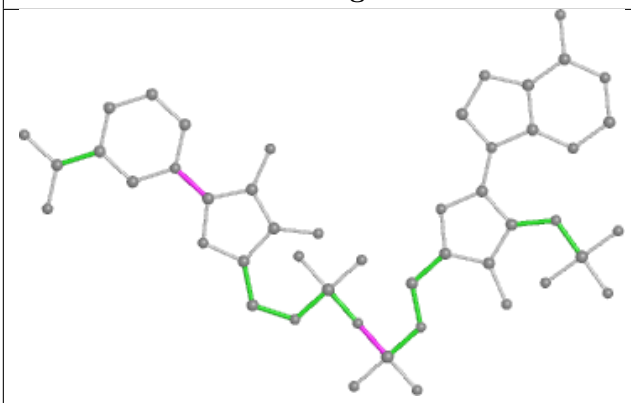

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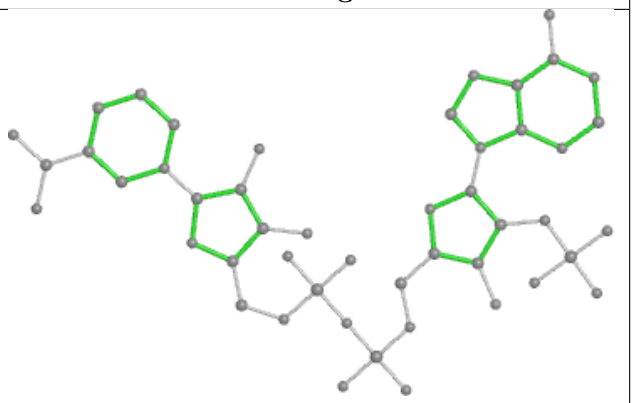
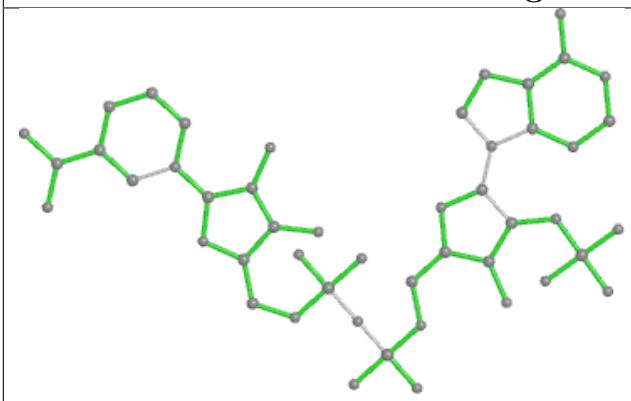


Rings

Ligand NDP J 401



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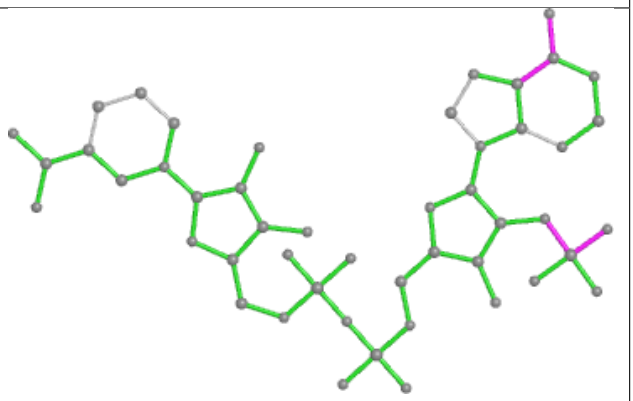
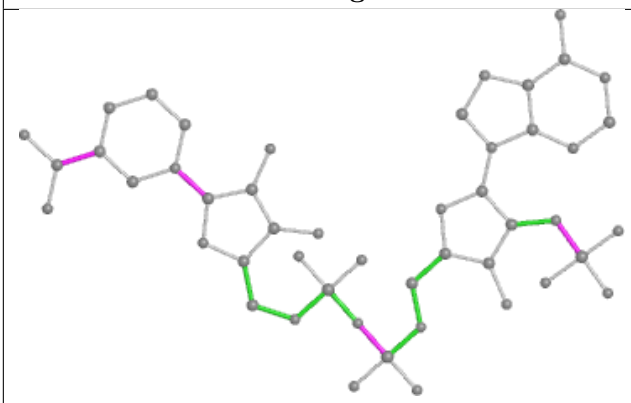


Bond angles



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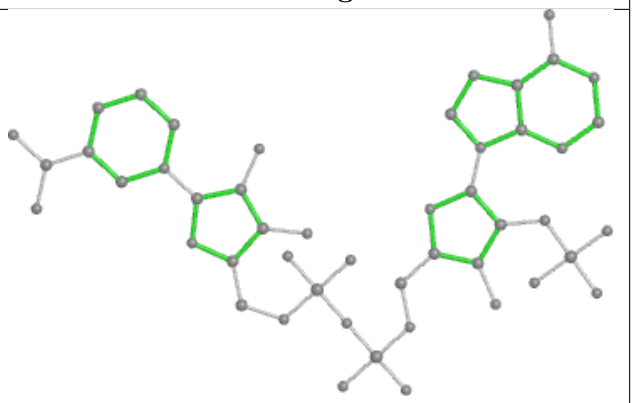
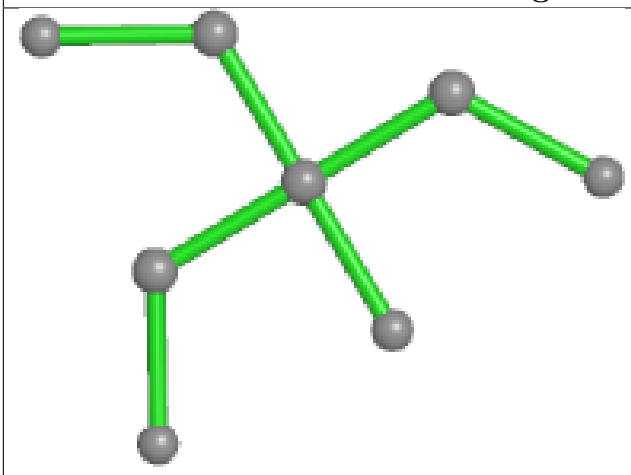
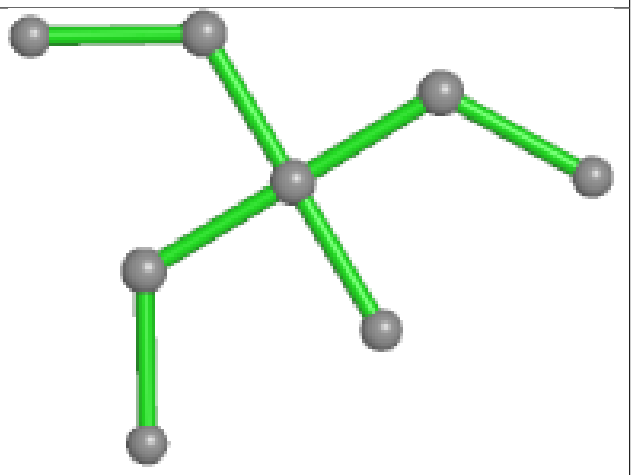


Rings

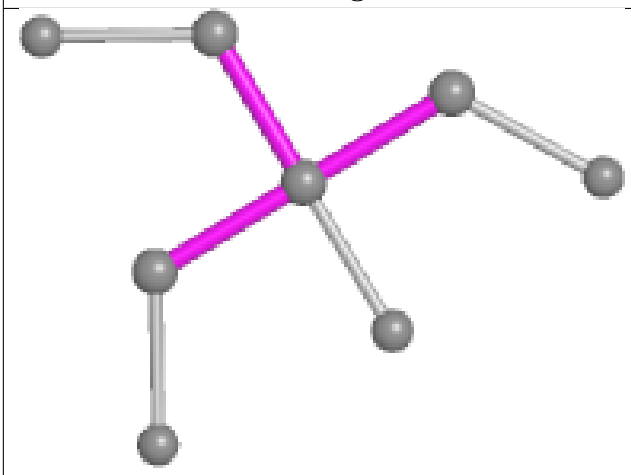
Ligand TRS I 401



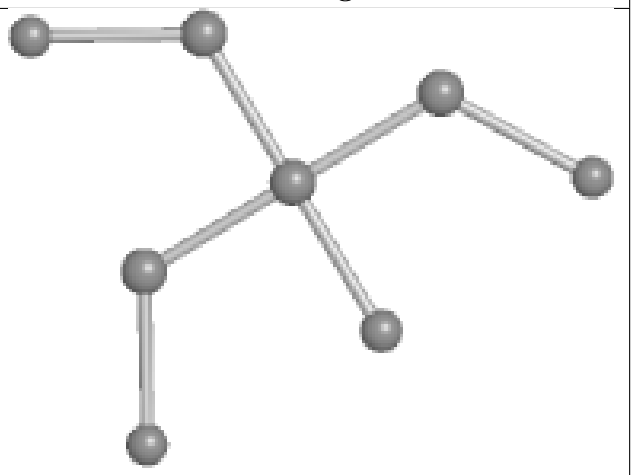
Bond lengths



Bond angles

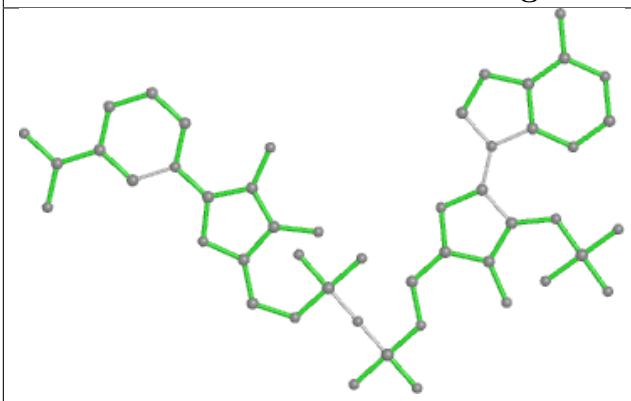


Torsions

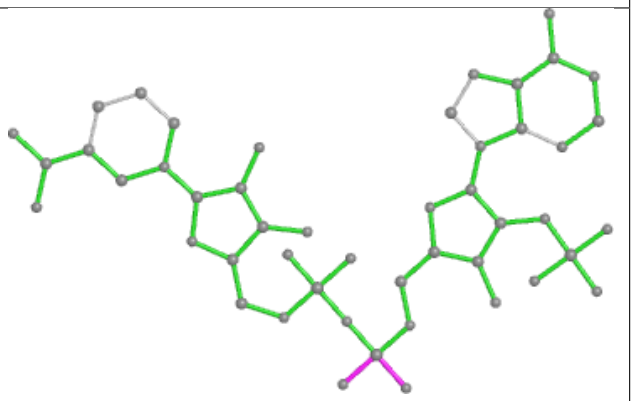


Rings

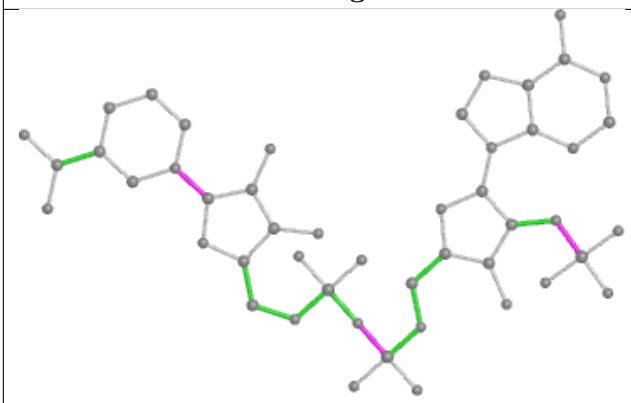
Ligand NDP D 401



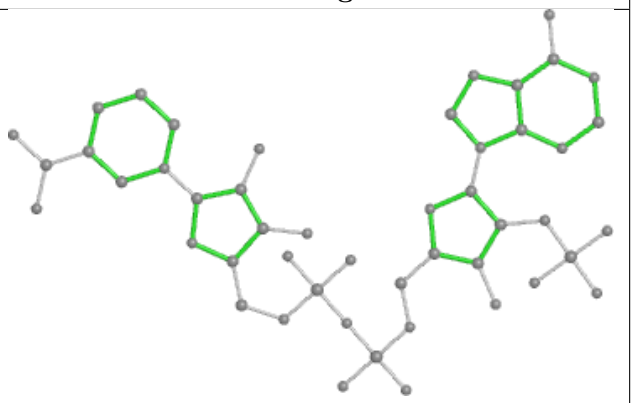
Bond lengths



Bond angles

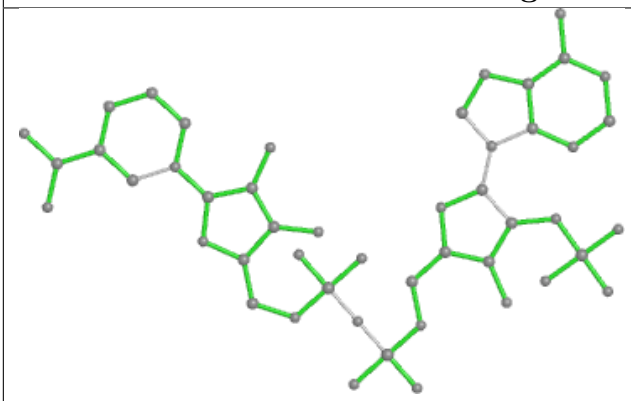


Torsions

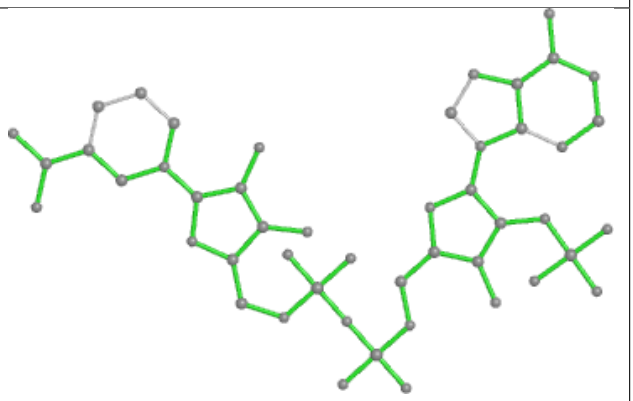


Rings

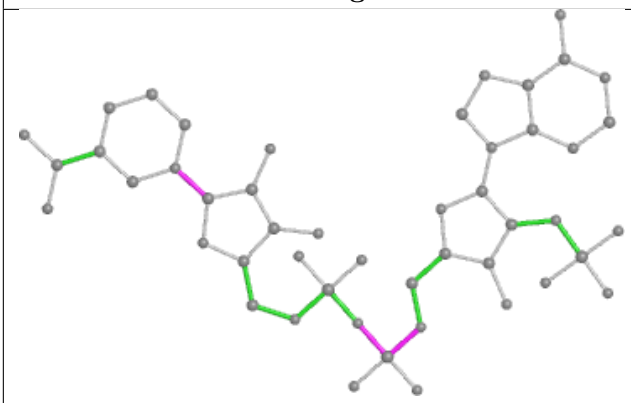
Ligand NDP H 401



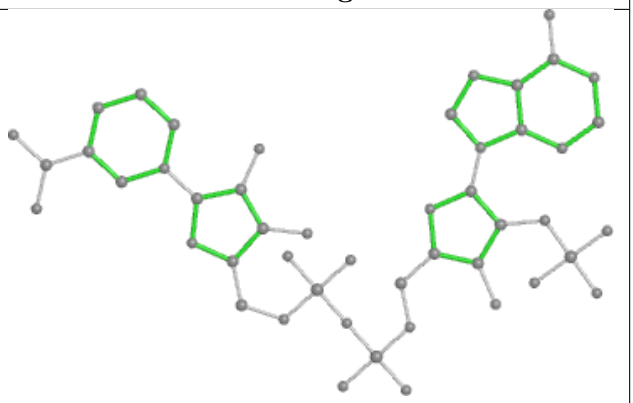
Bond lengths



Bond angles

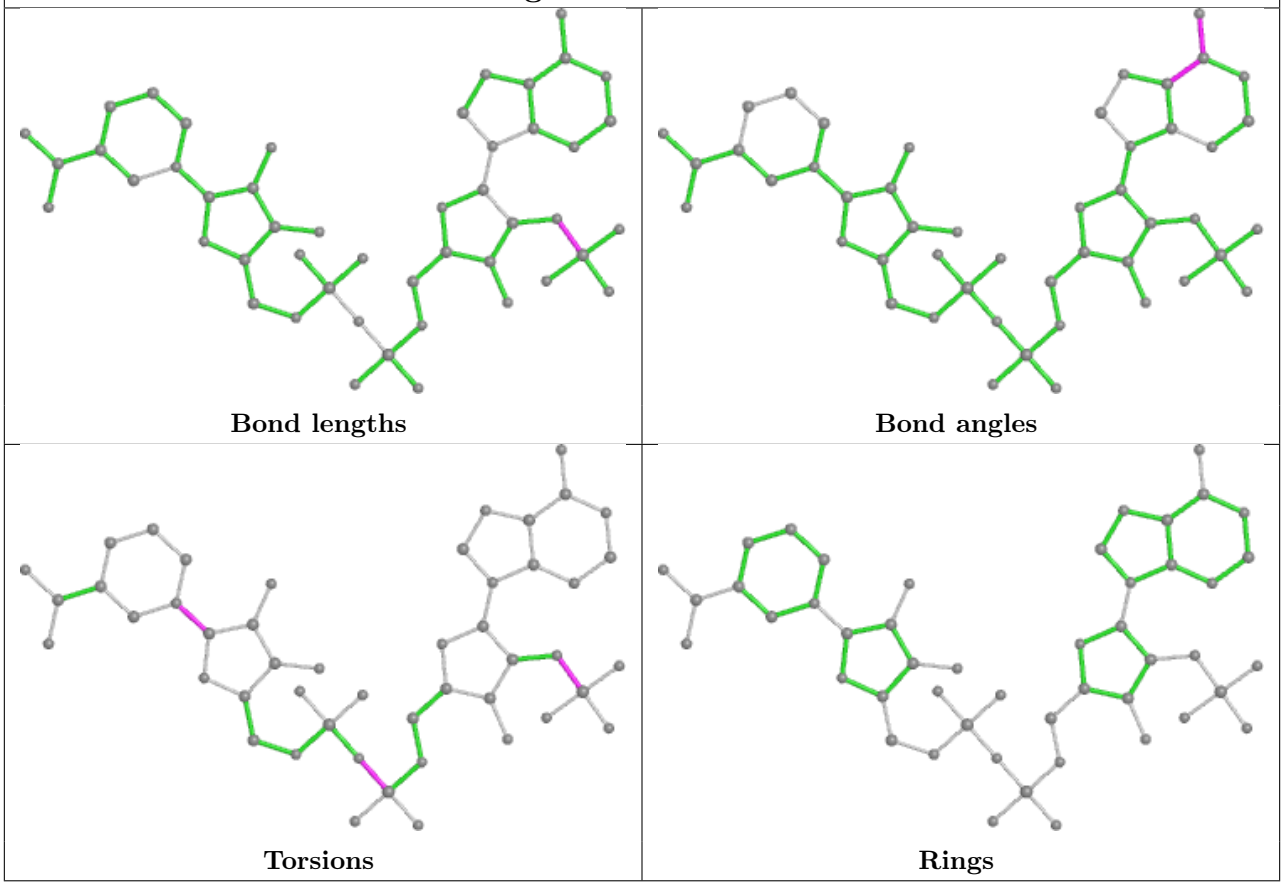


Torsions



Rings

Ligand NDP L 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	296/351 (84%)	0.09	21 (7%)	16	21	28, 50, 91, 116	0
1	B	312/351 (88%)	0.28	27 (8%)	10	14	28, 49, 89, 116	0
1	C	292/351 (83%)	0.30	30 (10%)	6	9	29, 53, 88, 115	0
1	D	314/351 (89%)	0.10	23 (7%)	15	20	25, 41, 85, 127	0
1	E	294/351 (83%)	0.14	21 (7%)	16	21	30, 50, 87, 109	0
1	F	313/351 (89%)	0.18	22 (7%)	16	22	28, 48, 85, 111	0
1	G	296/351 (84%)	0.14	17 (5%)	23	30	28, 47, 82, 113	0
1	H	307/351 (87%)	-0.02	13 (4%)	36	43	26, 41, 80, 114	0
1	I	300/351 (85%)	0.06	17 (5%)	23	30	23, 40, 80, 99	0
1	J	321/351 (91%)	-0.00	16 (4%)	28	36	22, 35, 76, 112	0
1	K	295/351 (84%)	-0.00	17 (5%)	23	29	24, 43, 76, 105	0
1	L	326/351 (92%)	-0.05	13 (3%)	38	45	22, 36, 71, 92	0
1	M	295/351 (84%)	-0.01	14 (4%)	31	38	24, 42, 81, 126	0
1	N	315/351 (89%)	-0.13	11 (3%)	44	51	24, 36, 70, 106	0
1	O	295/351 (84%)	0.05	10 (3%)	45	52	25, 41, 74, 101	0
1	P	330/351 (94%)	-0.04	14 (4%)	36	43	23, 33, 69, 93	0
All	All	4901/5616 (87%)	0.07	286 (5%)	23	29	22, 42, 82, 127	0

The worst 5 of 286 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	92	LEU	5.0
1	L	237	ALA	5.0
1	D	249	PRO	4.9
1	F	95	PRO	4.9
1	I	87	TYR	4.9

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

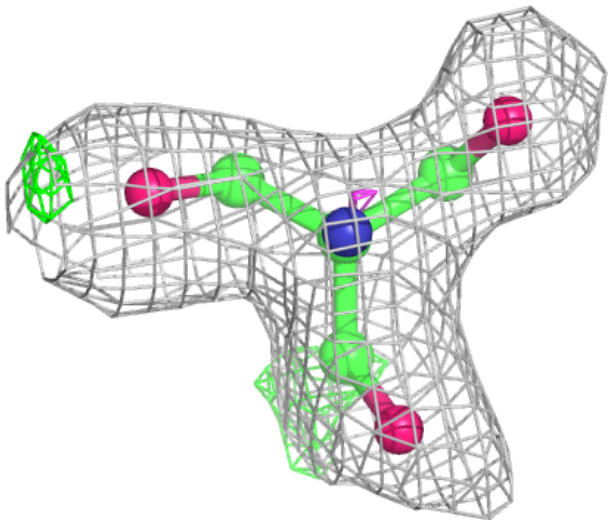
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

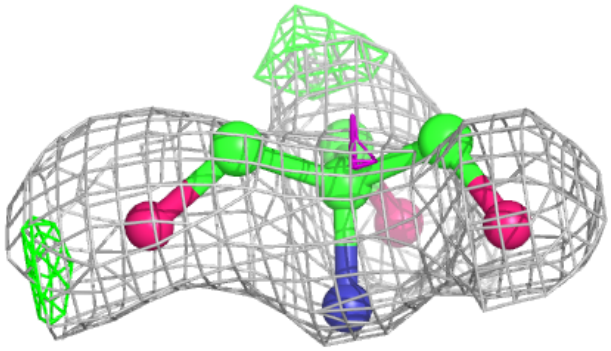
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	TRS	I	401	8/8	0.74	0.29	56,64,67,70	0
2	NDP	N	401	48/48	0.83	0.22	37,62,81,84	48
2	NDP	H	401	48/48	0.85	0.21	43,71,83,86	48
2	NDP	J	401	48/48	0.88	0.20	31,53,66,72	48
2	NDP	D	401	48/48	0.89	0.17	37,66,78,80	48
2	NDP	L	401	48/48	0.92	0.15	31,48,59,65	48
2	NDP	P	401	48/48	0.93	0.16	27,43,55,59	48

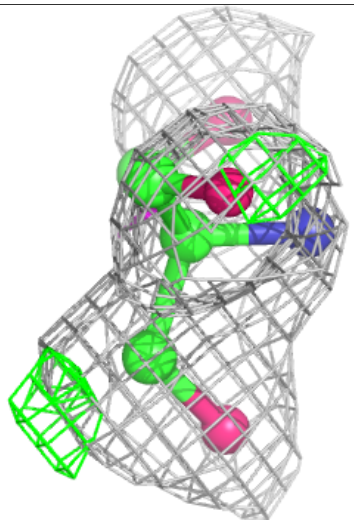
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around TRS I 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

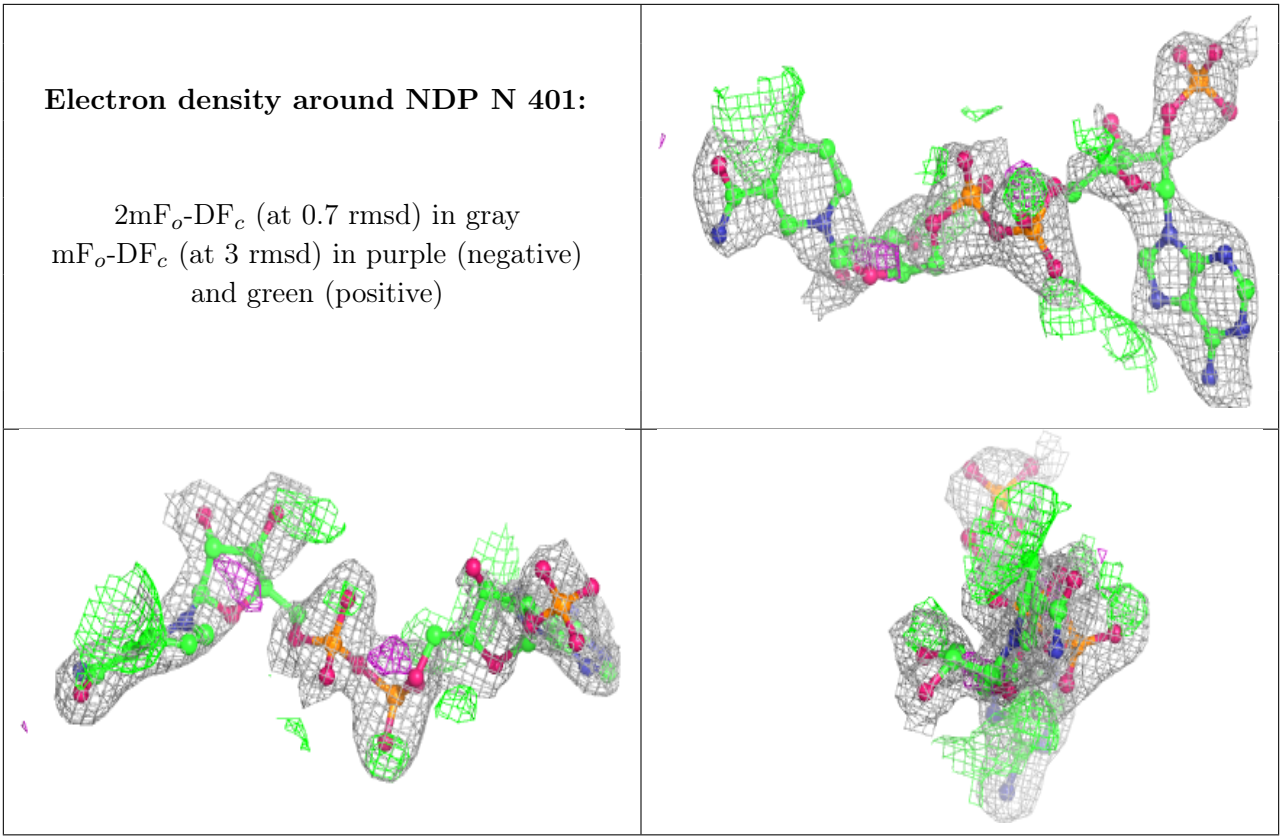






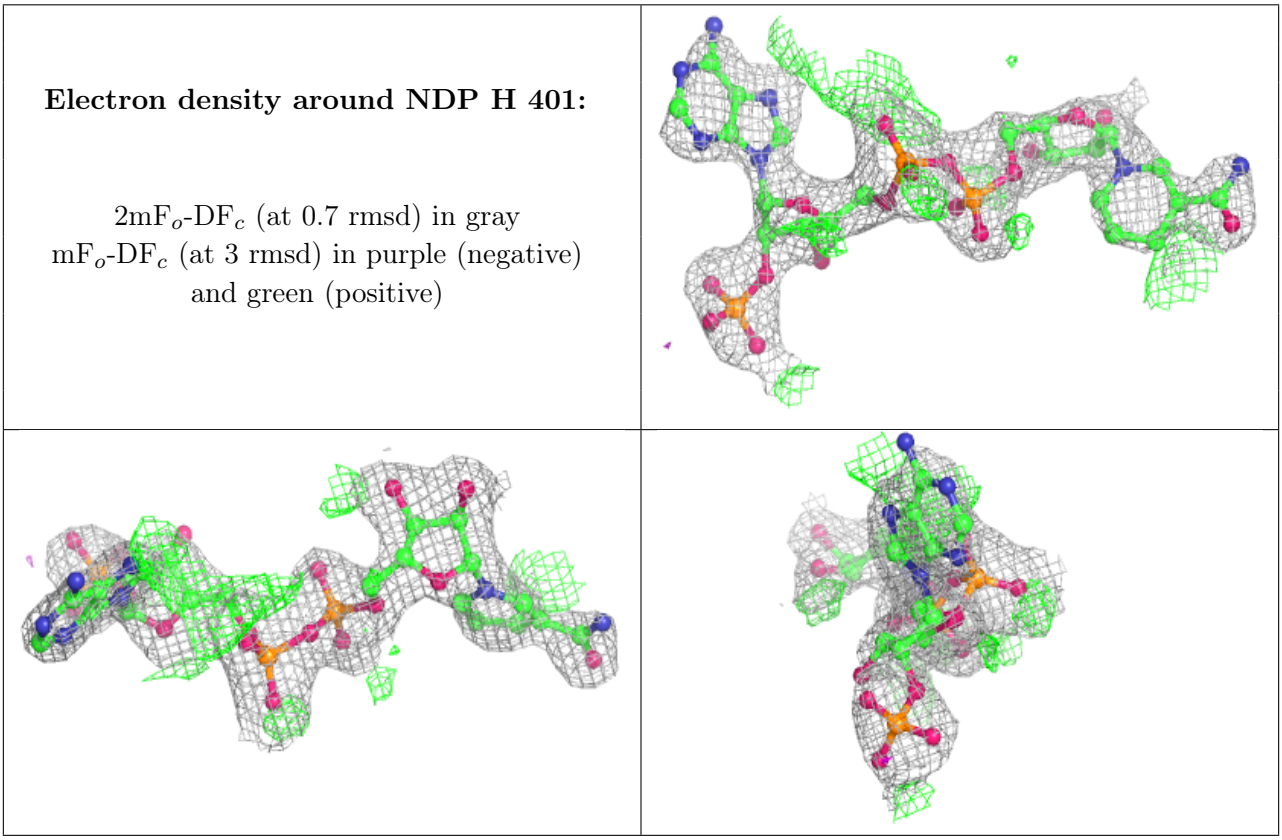
Electron density around NDP N 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



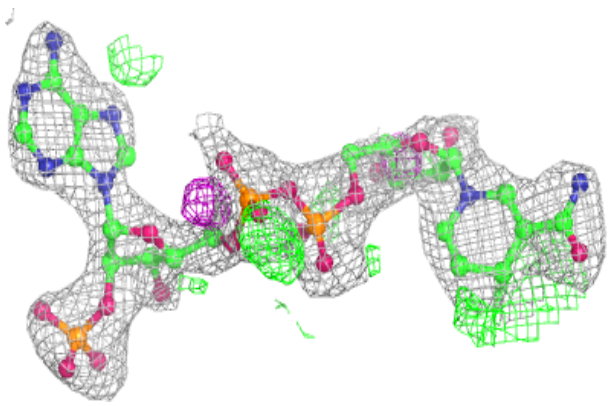
Electron density around NDP H 401:

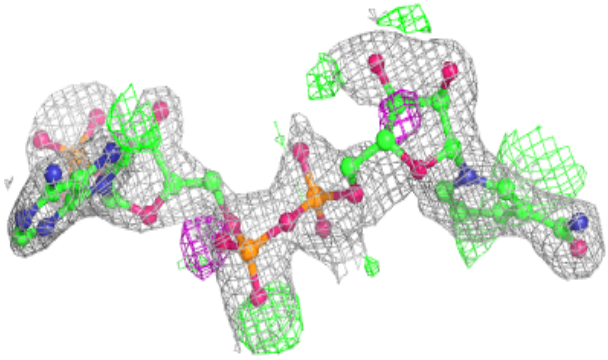
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

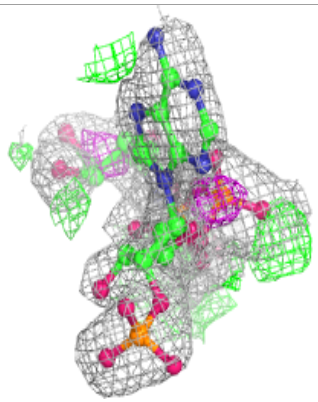


Electron density around NDP J 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

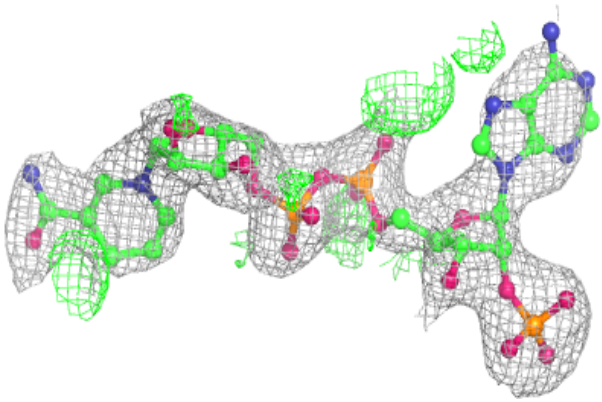


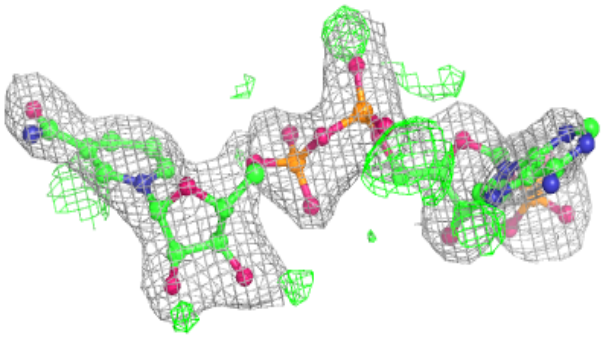


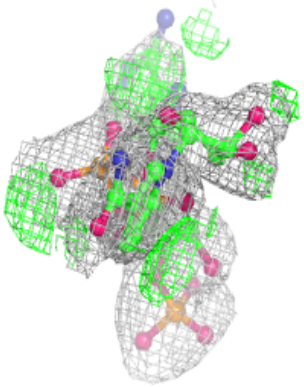


Electron density around NDP D 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

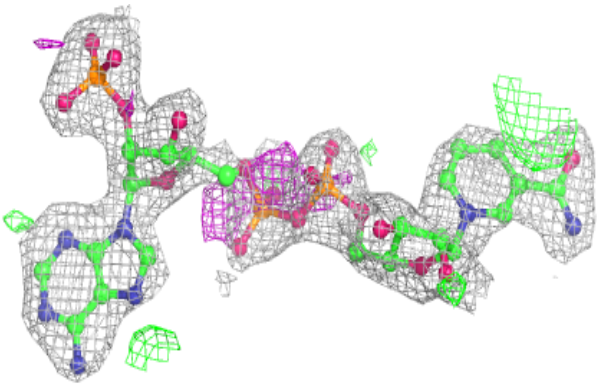


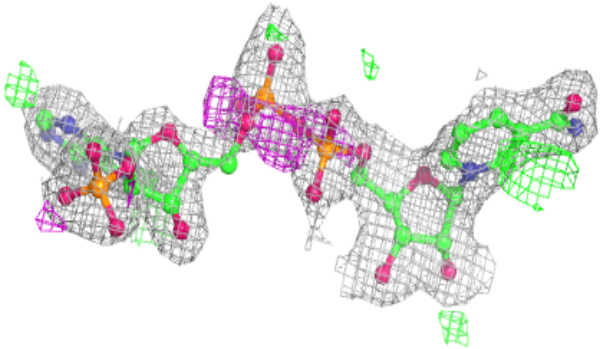


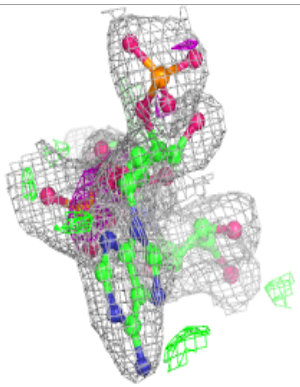


Electron density around NDP L 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

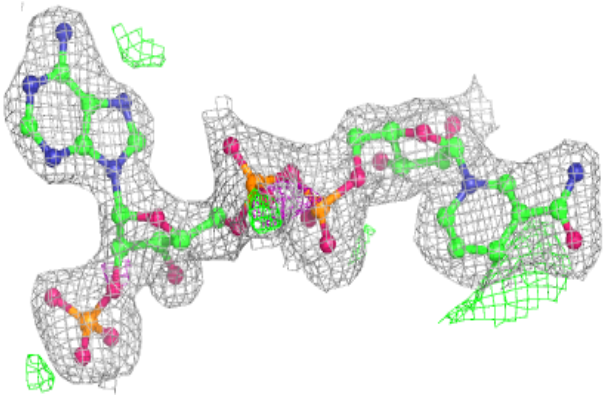


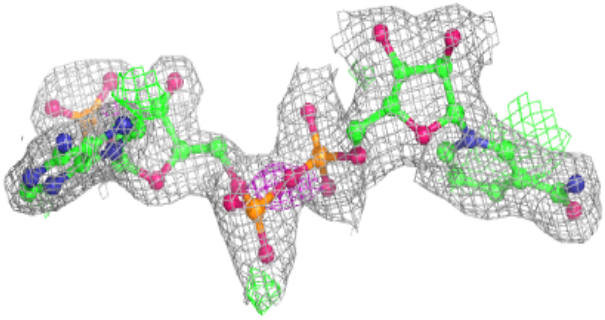


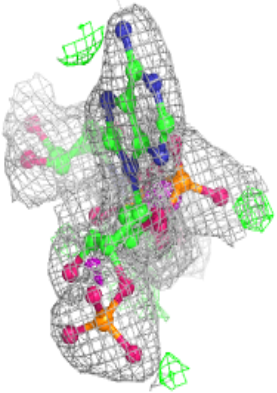


Electron density around NDP P 401:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.